AN ARGON-OXYGEN COVALENT BOND IN THE $ArOH^+$ MOLECULAR ION

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Although the OH^+ cation is decidedly a triplet ($^3\Sigma^-$) being over 50 kcal mol^{-1} more stable than the corresponding singlet ($^1\Delta$), binding to an argon atom can reverse this situation. The noble gas forms a strong donor-acceptor bond to the excited state singlet cation with a bond strength of 66.4 kcal mol^{-1} at the CCSDT(Q)/CBS level of theory. This makes the singlet 3.9 kcal mol^{-1} more stable than the most favorable triplet $Ar{-}HO^+$ complex. In a cold molecular beam experiment we have prepared both, singlet and triplet, isomers of this molecular ion depending on the employed ion source. Photodissociation spectroscopy in combination with messenger atom tagging reveals that the two observed spin isomers exhibit completely different spectral signatures in the infrared and the O−H stretching fundamentals differ by about 900 cm^{-1}. These findings might encourage the search for a new potential interstellar noble gas molecule.